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FILE COVERS 1907 - 17 Jul 2003 VOL 139 ISS 3 FILE LAST UPDATED: 16 Jul 2003 (20030716/ED)

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E CHINAREV A/AU L5 7 S E4-E8

E DICUSAR M/AU 1 S E4 L6

E GAMBARIAN A/AU E GAMBARIYAN A/AU

L7 1 S E4

E MARININA V/AU

11 S E4, E6 L8

230 S L3-L8 NOT L1 1.9

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L11 1116 S L10

11 S 3392-07-2 OR 29248-48-4 OR 51513-80-5 OR 53546-95-5 OR 137125 1.12

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           1108 S L11 NOT L2
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             53 S E3-E10
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                E GAMBARYAN A/AU
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L41 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS
     2001:792325 HCAPLUS
AN
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     135:313605
.TI
     Compounds, including saccharide compounds, for treatment of bacterial
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infections, and preparation thereof

- IN Bundle, David R.; Kitov, Pavel; Read, Randy J.; Ling, Hong; Armstrong, Glen
- PA Governors of the University of Alberta, Can.
- SO U.S., 47 pp., Cont.-in-part of U.S. 5,962,423.

CODEN: USXXAM

- DT Patent
- LA English
- IC ICM A61K031-70

ICS C12Q001-04

NCL 514025000

CC 1-5 (Pharmacology)

Section cross-reference(s): 33, 63

FAN.CNT 3

PATENT NO. KIND DATE	APPLICATION NO. DATE
PI US 6310043 B1 20011030	US 1999-317290 19990524 <
US 5962423 A 19991005	US 1998-130495 19980807
CA 2339198 AA 20000217	CA 1999-2339198 19990806
WO 2000008467 A2 20000217	WO 1999-CA725 19990806
WO 2000008467 A3 20000706	
W: AU, CA, JP	
	FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE	1000 51450 1000006
AU 9951450 A1 20000228	AU .1999-51450 19990806
AU 754331 B2 20021114	ED 1000 036010 1000006
<del></del>	EP 1999-936219 19990806
, , ,	GB, GR, IT, LI, LU, NL, SE, MC, PT,
.IE, FI PRAI US 1998-130495 A2 19980807	
US 1999-317290 A 19990524	•

WO 1999-CA725 W 19990806 Compds. which bind to toxins assocd. with enteric bacterial infection, AB compns. including the compds., methods for the neutralization of toxins in a patient, and methods for the diagnosis of bacterial and viral infections are disclosed. Toxins which can be bound by the compds. include pentameric toxins, for example SLTs (shiga-like toxins), such as those from Salmonella, Campylobacter and other bacteria, verotoxins from E. coli, cholera toxin, Clostridium difficile toxins A and B, bacterial pili from enteropathogenic E. coli and enterotoxigenic E. coli and viral lectins, such as viral hemagglutinins. The compds. include a core mol. bound to a plurality of linker arms, which in turn are bound to a plurality of bridging moieties, which in turn are bound to at least one, and preferably, two or more ligands which bind to the toxin. Examples of suitable ligands include di- and for trisaccharide moieties. The di- or tri-saccharide moieties themselves are active in binding to the SLTs. presence of a plurality of bridged dimers of the ligands is responsible for the increased binding affinity of the compds. relative to the ligands themselves. In one embodiment, the compds., when administered in a timely fashion to a patient suffering from enteric E. coli infection, inhibit progression of this infection into hemolytic uremic syndrome (HUS).

ST dendrimer oligosaccharide Prepn antibacterial; antibacterial bacterial toxin saccharide deriv prepn; bacteria virus infection diagnosis; Escherichia hemolytic uremic syndrome saccharide deriv

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(B, Clostridium difficile; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL

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infections, and prepn. thereof)

(Biological study) (Shiga-like toxin I; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Toxins RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (Shiga-like toxin II; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Toxins RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (Shiga-like toxin; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Carbohydrates, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) (aldaric acids; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Peptides, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) (amino acids; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Infection (bacterial, diagnosis; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Toxins RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (cholera; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Antibacterial agents Campylobacter Drug delivery systems Salmonella (compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Toxins RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Dendritic polymers RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Agglutinins and Lectins RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Amino acids, biological studies Disaccharides Monosaccharides Oligosaccharides, biological studies Trisaccharides RL: BSU (Biological study, unclassified); BIOL (Biological study) (compds., including saccharide compds., for treatment of bacterial

IT Escherichia coli (enterotoxigenic; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) IΤ Pilus (from enteropathogenic E. coli; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) IT Drug delivery systems (injections; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ΙT Fluorescent substances (label; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) Enzymes, biological studies ΙT Radionuclides, biological studies RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (label; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ΙT Drug delivery systems (oral; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ΙT Intestinal bacteria (pathogenic, pili from enteropathogenic E. coli; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ΙT Escherichia coli (pili from enteropathogenic E. coli; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ITAlcohols, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) (polyhydric; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ITAlbumins, biological studies RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (saccharide derivs.; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ΙT Toxins RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (toxin A, Clostridium difficile; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) IT Clostridium difficile (toxins A and B; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) ΙT (viral lectin; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) 258873-66-4P IΤ RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof) 79-06-1D, Acrylamide, derivs. 574-93-6D, Phthalocyanine, derivs. 12619-70-4D, Cyclodextrin, derivs. 13117-26-5D derivs. 54832-51-8D, derivs. 66580-68-5D, derivs. RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compds., including saccharide compds., for treatment of bacterial

IT 58-85-5 9013-20-1, Streptavidin

infections, and prepn. thereof)

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RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (label; compds., including saccharide compds., for treatment of
        bacterial infections, and prepn. thereof)
ΙT
     244076-91-3P 244076-92-4P 244076-93-5P
     244076-96-8P 244076-97-9P 244076-98-0P
     244076-99-1P 244077-00-7P 244077-01-8P
     244077-02-9P 244077-03-0P 244077-04-1P
     244077-05-2P 244077-06-3P 244077-07-4P
     244077-08-5P 244077-09-6P 258857-10-2P
     258857-11-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction; compds., including saccharide compds., for
        treatment of bacterial infections, and prepn. thereof)
IT
     98-88-4, Benzoyl chloride 100-39-0 106-95-6,
     Allyl bromide, reactions 107-15-3, 1,2-Ethanediamine, reactions
     373-44-4, 1,8-Octanediamine 616-29-5,
     1,3-Diamino-2-hydroxypropane 1125-88-8 2365-48-2,
     Methyl thioglycolate 5231-87-8 7693-46-1,
     4-Nitrophenyl chloroformate 41110-63-8 63976-06-7
     102674-58-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction; compds., including saccharide compds., for treatment of
        bacterial infections, and prepn. thereof)
              THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
        104
RE
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- IT 258873-66-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BFOL (Biological study); PREP (Preparation); USES (Uses)

(compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

- RN 258873-66-4 HCAPLUS
- CN Carbamic acid, [.beta.-D-glucopyranose-1,2,3,4,6-penta-O-ylpentakis[3,1-propanediylthio(1-oxo-2,1-ethanediyl)imino-2,1-ethanediylimino(3,4-dioxo-1-cyclobutene-2,1-diyl)imino-8,1-octanediyliminocarbonyloxy-3,1,2-propanetriyl]]decakis-, decaester with methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-(2-hydroxyethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-.beta.-D-glucopyranoside (9CI) (CA INDEX NAME)
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- TT 79-06-1D, Acrylamide, derivs. 574-93-6D, Phthalocyanine,
   derivs. 12619-70-4D, Cyclodextrin, derivs. 13117-26-5D
   , derivs. 54832-51-8D, derivs. 66580-68-5D, derivs.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

- RN 79-06-1 HCAPLUS
- CN 2-Propenamide (9CI) (CA INDEX NAME)

RN 574-93-6 HCAPLUS

CN 29H, 31H-Phthalocyanine (9CI) (CA INDEX NAME)

RN 12619-70-4 HCAPLUS

CN Cyclodextrin (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 13117-26-5 HCAPLUS

CN D-Galactose, 4-O-.alpha.-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 54832-51-8 HCAPLUS

CN D-Glucose, O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 66580-68-5 HCAPLUS

CN D-Glucose, O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 58-85-5 9013-20-1, Streptavidin

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (label; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

RN 58-85-5 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 9013-20-1 HCAPLUS

r.

CN Streptavidin (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 244076-91-3P 244076-92-4P 244076-93-5P 244076-96-8P 244076-97-9P 244076-98-0P 244076-99-1P 244077-00-7P 244077-01-8P

244077-02-9P 244077-03-0P 244077-04-1P

244077-05-2P 244077-06-3P 244077-07-4P 244077-08-5P 244077-09-6P 258857-10-2P

258857-11-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

RN 244076-91-3 HCAPLUS

CN D-Glucopyranose, 4-0-(3,4,6-tri-0-acetyl-2-0-2-propenyl-.beta.-D-galactopyranosyl)-, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244076-92-4 HCAPLUS

CN .alpha.-D-Glucopyranosyl chloride, 4-O-(3,4,6-tri-O-acetyl-2-O-2-propenyl-beta.-D-galactopyranosyl)-, triacetate (9CI) (CA INDEX NAME)

RN 244076-93-5 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-(2-O-2-propenyl-.beta.-D-galactopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 244076-96-8 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 2,3,6-tris-O-(phenylmethyl)-4-O-[3-O-(phenylmethyl)-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-97-9 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-[6-O-benzoyl-3-O-(phenylmethyl)-2-O-2-propenyl-.beta.-D-galactopyranosyl]-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 244076-98-0 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-6-O-benzoyl-3-O-(phenylmethyl)-2O-2-propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244076-99-1 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3-O-(phenylmethyl)-2-O-2propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-00-7 HCAPLUS

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CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-2-O-2propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 244077-01-8 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-(2-hydroxyethyl)-3,6-bis-O(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-02-9 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-[2-[[(4-nitrophenoxy)carbonyl]oxy]ethyl]-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 244077-03-0 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[(2-hydroxy-1,3-propanediyl)bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 2-B

RN 244077-04-1 HCAPLUS

.beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[(4-nitrophenoxy)carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 2-A

O Ph

PAGE 2-B

Ph O

RN 244077-05-2 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[(8-aminooctyl)amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

PAGE 2-B

.... OMe

Ph

PAGE 3-B

Ph

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[(8-aminooctyl)amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

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PAGE 1-A

PAGE 1-B

ОН

PAGE 2-A

PAGE 2-B

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<u>r</u>.

RN 244077-07-4 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[[8-[(2-ethoxy-3,4-dioxo-1-cyclobuten-1-yl)amino]octyl]amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 2-B

HO

RN 244077-08-5 HCAPLUS

CN Acetic acid, [[3-[[2,3,4,6-tetrakis-O-[3-[(2-methoxy-2-oxoethyl)thio]propyl]-.beta.-D-glucopyranosyl]oxy]propyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244077-09-6 HCAPLUS

二

CN Acetamide, N-(2-aminoethyl)-2-[[3-[[2,3,4,6-tetrakis-O-[3-[[2-[(2-aminoethyl)amino]-2-oxoethyl]thio]propyl]-.beta.-D-

glucopyranosyl]oxy]propyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B

RN 258857-10-2 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-[4,6-O-(phenylmethylene)-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 258857-11-3 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 2,3,6-tris-O-(phenylmethyl)-4-O-[3-O-(phenylmethyl)-4,6-O-(phenylmethylene)-2-O-2-propenyl-.beta.-D-

galactopyranosyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 98-88-4, Benzoyl chloride 100-39-0 106-95-6,
 Allyl bromide, reactions 107-15-3, 1,2-Ethanediamine, reactions
 373-44-4, 1,8-Octanediamine 616-29-5,
 1,3-Diamino-2-hydroxypropane 1125-88-8 2365-48-2,
 Methyl thioglycolate 5231-87-8 7693-46-1,
 4-Nitrophenyl chloroformate 41110-63-8 63976-06-7
 102674-58-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)
RN 98-88-4 HCAPLUS
CN Benzoyl chloride (8CI, 9CI) (CA INDEX NAME)

RN 100-39-0 HCAPLUS CN Benzene, (bromomethyl)- (9CI) (CA INDEX NAME)

Ph-CH2-Br

RN 106-95-6 HCAPLUS CN 1-Propene, 3-bromo- (9CI) (CA INDEX NAME)

Br-CH2-CH=CH2

RN 107-15-3 HCAPLUS CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

RN 373-44-4 HCAPLUS

CN 1,8-Octanediamine (6CI, 8CI, 9CI) (CA INDEX NAME)

 $H_2N-(CH_2)_8-NH_2$ 

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RN 616-29-5 HCAPLUS

CN 2-Propanol, 1,3-diamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 1125-88-8 HCAPLUS

CN Benzene, (dimethoxymethyl) - (9CI) (CA INDEX NAME)

RN 2365-48-2 HCAPLUS

CN Acetic acid, mercapto-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 5231-87-8 HCAPLUS

CN 3-Cyclobutene-1,2-dione, 3,4-diethoxy- (9CI) (CA INDEX NAME)

RN 7693-46-1 HCAPLUS

CN Carbonochloridic acid, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

RN 41110-63-8 HCAPLUS

CN .alpha.-D-Galactopyranosyl chloride, 2,3,4,6-tetrakis-O-(phenylmethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 63976-06-7 HCAPLUS

CN .beta.-D-Glucopyranoside, 2-propenyl 2,3,4,6-tetra-O-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2C$$
 $O$ 
 $R$ 
 $R$ 
 $O$ 
 $CH_2$ 

RN 102674-58-8 HCAPLUS

CN D-Glucose, 4-O-[6-O-(1-methoxy-1-methylethyl)-3,4-O-(1-methylethylidene)-.beta.-D-galactopyranosyl]-2,3:5,6-bis-O-(1-methylethylidene)-, dimethyl acetal (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L41 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS

AN 2001:31361 HCAPLUS

DN 134:101139

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TI Preparation of self-associating compounds and their aggregate bodies for use as medicaments

IN Bovin, Nikolai Vladimirovich; Tusikov, Alexandr Borisovich; Chinarev, Alexandr Alexandrovich; Dicusar, Mariya Alexandrovna; Gambariyan, Alexandra Sergeevna;

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Marinina, Valentina Petrovna
PΑ
     Syntesome Gesellschaft fur Medizinische Biochemie m.b.H., Germany
SO
     PCT Int. Appl., 60 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     German
IC
     ICM A61K047-48
CC
     33-4 (Carbohydrates)
     Section cross-reference(s): 34, 63
FAN.CNT 1
     PATENT NO.
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                                           APPLICATION NO.
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                                           WO 2000-EP6139
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PΙ
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     WO 2001002018
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             IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
             MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
             SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
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                            20010111
                                           DE 1999-19930177 19990630 <--
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                            20020724
                                           EP 2000-949235
                                                           20000630 <--
     EP 1223984
                       A2
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
     JP 2003503465
                       Т2
                            20030128
                                           JP 2001-507508
                                                            20000630 <--
PRAI DE 1999-19930177
                      Α
                            19990630
                                      <--
     WO 2000-EP6139
                       W
                            20000630
                                     <--
     Title compds., [e.g., {.alpha.-Neu5Ac-OCH2-4-C6H4-
AB
     NHC(0)CH2NHC(0)(CH2)4C(0)(NHCH2C(0))0-7NHCH2\}4C, in which the terminal
     portion of each arm may contain fragments capable of cellular receptor
     blocking, antibiotic, or therapeutic action, capable of forming
     self-aggregates, were prepd. for use as drug-delivery or diagnostic
     agents. The tetrahedral core was synthesized from {H2NCH2}4C using
     BOC-peptide coupling chem. The terminal units were prepd. from
     tetra-O-acetyl-5-acetylneuraminic acid Me ester derivs.,
     5-acetylneuraminic acid .alpha.-2.fwdarw.3-B-D-GalP-(1.fwdarw.4)-.beta.-D-
     GluP-NHC(O)CH2NH2, or .alpha.-D-GalP-(1.fwdarw.3)-.beta.-D-GalP-O-
     (CH2)3NH2 derivs. In a test of inhibition of viral cell adhesion, using
     influenza virus, {.alpha.-Neu5Ac-OCH2-4-C6H4-NHC(O)CH2NHC(O)(CH2)4C(O)(NH(
     CH2)5C(O))3(NHCH2C(O))5NHCH2}4C had relative activity (to
     Neu5Ac-.alpha.-CH2Ph) of 2500:1.
ST
     oligosaccharide peptide conjugate prepn aggregating drug delivery
ΙT
     Neoplasm.
        (metastasis; prepn. of self-assocg. compds. and their aggregate bodies
        for use as medicaments)
ΙT
     Autoimmune disease
     Coupling reaction
     Drug delivery systems
     Infection
     Inflammation
     Influenza virus
     Self-association
        (prepn. of self-assocq. compds. and their aggregate bodies for use as
        medicaments)
ΙT
     Transplant and Transplantation
        (rejection; prepn. of self-assocg. compds. and their aggregate bodies
        for use as medicaments)
ΙT
     Wound healing
        (selectin-facilitated; prepn. of self-assocg. compds. and their
        aggregate bodies for use as medicaments)
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318286-47-4P 318286-49-6P 318286-51-0P
TT
    318286-53-2P 318286-55-4P 318286-65-6DP,
    self-aggregates 318507-77-6P 318508-09-7P
    318508-48-4P 318508-50-8P 318508-52-0P
    318508-53-1DP, self-aggregates 318508-54-2DP,
    self-aggregates 318508-57-5DP, self-aggregates
    318508-58-6DP, self-aggregates 318509-04-5P
    318509-46-5P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of self-assocg. compds. and their aggregate bodies for use as
        medicaments)
ΙT
    3392-07-2 29248-48-4 51513-80-5
    53546-95-5 137125-82-7 201667-63-2
    205753-10-2 318286-06-5 318286-10-1
    318286-61-2 318286-67-8
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of self-assocg. compds. and their aggregate bodies for use as
        medicaments)
    14302-75-1P 32564-25-3P 205753-09-9P
    226408-84-0P 318285-90-4P 318285-93-7P
    318285-95-9P 318286-08-7P 318286-16-7P
    318286-19-0P 318286-21-4P 318286-23-6P
    318286-25-8P 318286-27-0P 318286-29-2P
    318286-31-6P 318286-33-8P 318286-35-0P
    318286-37-2P 318286-41-8P 318286-43-0P
    318286-57-6P 318286-59-8P 318286-69-0P
    318510-95-1P 318511-00-1P 318511-08-9P
    318511-10-3P 318511-11-4P 318511-17-0P
    318511-35-2P 318511-41-0P 318511-44-3P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of self-assocg. compds. and their aggregate bodies for use as
        medicaments)
    318285-97-1P 318285-99-3P 318286-01-0P
IT
    318286-03-2P 318286-45-2P 318286-63-4P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of self-assocg. compds. and their aggregate bodies for use as
        medicaments)
IT
    318286-47-4P 318286-49-6P 318286-51-0P
    318286-53-2P 318286-55-4P 318286-65-6DP,
    self-aggregates 318507-77-6P 318508-09-7P
    318508-48-4P 318508-50-8P 318508-52-0P
    318508-53-1DP, self-aggregates 318508-54-2DP,
    self-aggregates 318508-57-5DP, self-aggregates
    318508-58-6DP, self-aggregates 318509-04-5P
    318509-46-5P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of self-assocg. compds. and their aggregate bodies for use as
        medicaments)
RN
    318286-47-4 HCAPLUS
CN ·
     .alpha.-Neuraminic acid, 2,2'-O-[[15,15-bis[[[[6-[[2-[[4-[[(N-acetyl-
     .alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-
    dioxohexyl]amino]acetyl]amino]methyl]-1,4,9,12,18,21,16,29-octaoxo-
     3,10,13,17,20,27-hexaazanonacosane-1,29-diyl]bis(imino-4,1-
    phenylenemethylene)]bis[N-acetyl- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$\begin{array}{c|c}
R \\
H \\
NH \\
O\end{array}$$

$$\begin{array}{c}
H \\
NH \\
O\end{array}$$

$$\begin{array}{c}
O \\
CH_2
\end{array}$$

$$\begin{array}{c}
H \\
HN \\
HN\end{array}$$

PAGE 1-C

со<sub>2</sub>н

PAGE 2-A

PAGE 2-C

PAGE 3-A

RN 318286-49-6 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]a mino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycyl-, 2,2',2'',2'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-C

PAGE 3-A

PAGE 3-B

RN 318286-51-0 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]a mino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycyl-, 3,3',3'',3''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-A

PAGE 2-C

PAGE 3-A

PAGE 3-B

RN 318286-53-2 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]a mino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycylglycyl-, 4,4',4'',4'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$\begin{array}{c|c} & & & & \\ & &$$

# PAGE 1-C

## PAGE 1-D

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23E

PAGE 3-A

PAGE 3-B

RN 318286-55-4 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]a mino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycylglycylglycyl-, 5,5',5'',5'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

$$\begin{array}{c|c} H \\ N \\ O \\ \end{array}$$

PAGE 1-D

PAGE 2-A

PAGE 2-D

PAGE 3-B

RN 318286-65-6 HCAPLUS

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CN Glycinamide, 6,6'-(1,4-butanediyl)bis[N-[6-[[2-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycy

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$-\frac{H}{N}$$

$$\frac{H}{N}$$

$$\frac{H$$

PAGE 1-C

PAGE 1-D

RN 318507-77-6 HCAPLUS

Glycine, N-[6-[[6-[[2-[[4-[[(N-acetyl-.alpha.neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6dioxohexyl]amino]-1-oxohexyl]amino]-1-oxohexyl]glycylglycylglycylglycyl-,
5,5',5'',5'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine
(9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318508-09-7 HCAPLUS

CN Glycine, N-[30-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amin o]-1,8,15,22,27,30-hexaoxo-7,14,21,28-tetraazatriacont-1-yl]glycylglycylglycylglycyl-, 5,5',5'',5'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318508-48-4 HCAPLUS

CN Glycine, N-[6-[[6-[[2-[[4-[[(N-acetyl-.alpha.neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-6-oxohexyl]amino]1,6-dioxohexyl]glycylglycylglycylglycyl-, 5,5',5'',5'''-tetraamide with
2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318508-50-8 HCAPLUS

```
CN
     Glycine, N-[6-[[6-[[6-[[4-[[4-[[(N-acetyl-.alpha.-
     neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-6-oxohexyl]amino]-
     6-oxohexyl]amino]-1,6-dioxohexyl]glycylglycylglycylglycyl-,
     5,5',5'',5'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine
     (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     318508-52-0 HCAPLUS
RN
CN
     Glycine, N-[30-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amin
     o]-1,6,13,20,27,30-hexaoxo-7,14,21,28-tetraazatriacont-1-
     yl]glycylglycylglycylglycyl-, 5,5',5'',5'''-tetraamide with
     2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN
     318508-53-1 HCAPLUS
CN
     Glycine, N-[6-[[2-[[4-[[(N-acetyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]a
     mino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycylglycylglycylglycy
     1-, 7,7',7'',7'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine
     (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     318508-54-2 HCAPLUS
RN
     Glycine, N-[31-[(3-O-.alpha.-D-galactopyranosyl-.beta.-D-
CN
     galactopyranosyl)oxy]-1,8,15,22,27-pentaoxo-7,14,21,28-tetraazahentriacont-
     1-yl]glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-
     propanediamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     318508-57-5 HCAPLUS
RN
CN
     Glycine, N-[6-[[2-[[0-(N-acetyl-4,7,8,9-tetra-0-acetyl-.alpha.-
     neuraminosyl)-(2.fwdarw.3)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-.beta.-
     D-glucopyranosyl]amino]-2-oxoethyl]amino]-1,6-
     dioxohexyl]glycylglycylglycylglycyl-, 5,5',5'',5'''-tetraamide with
     2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN
     318508-58-6 HCAPLUS
     Glycine, N-[6-[[2-[[0-(N-acetyl-4,7,8,9-tetra-0-acetyl-.alpha.-
CN
     neuraminosyl)-(2.fwdarw.3)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-.beta.-
     D-glucopyranosyl]amino]-2-oxoethyl]amino]-1,6-
     dioxohexyl]glycylglycylglycylglycylglycylglycyl-, 7,7',7''-tetraamide
     with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     318509-04-5 HCAPLUS
RN
     Glycine, N-[6-[3-[0-(N-acetyl-4,7,8,9-tetra-0-acetyl-.alpha.-
CN
     neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-
     (acetylamino) -2-deoxy-.beta.-D-glucopyranosyl]oxy]propyl]amino]-1,6-
     \verb|dioxohexyl|| \verb|glycylglycylglycylglycylglycylglycyl-|, 7,7',7'',7'''-tetraamide|
     with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN
     318509-46-5 HCAPLUS
CN
     Glycine, N-[6-[6-[6-[3-[0-(N-acetyl-4,7,8,9-tetra-0-acetyl-.alpha.-
     neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-
     (acetylamino)-2-deoxy-.beta.-D-glucopyranosyl]oxy]propyl]amino]-1,6-
     dioxohexyl]amino]-1-oxohexyl]amino]-1-oxohexyl]glycylglycylglycylgly
     cylglycyl-, 7,7',7'',7'''-tetraamide with 2,2-bis(aminomethyl)-1,3-
     propanediamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
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TΤ

3392-07-2 29248-48-4 51513-80-5 53546-95-5 137125-82-7 201667-63-2

205753-10-2 318286-06-5 318286-10-1

318286-61-2 318286-67-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of self-assocg. compds. and their aggregate bodies for use as
 medicaments)

RN 3392-07-2 HCAPLUS

CN Carbamic acid, [2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 29248-48-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[N-[(1,1-dimethylethoxy)carbonyl]glycylglycyl]oxy ]- (9CI) (CA INDEX NAME)

RN 51513-80-5 HCAPLUS

CN Carbamic acid, [6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 53546-95-5 HCAPLUS

CN Hexanoic acid, 6-[[(1,1-dimethylethoxy)carbonyl]amino]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

RN 137125-82-7 HCAPLUS

CN .alpha.-Neuraminic acid, N-acetyl-2-0-[[4-[[[(1,1-

dimethylethoxy)carbonyl]amino]acetyl]amino]phenyl]methyl]-, methyl ester,
4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 201667-63-2 HCAPLUS

CN .beta.-D-Galactopyranoside, 3-aminopropyl 3-O-.alpha.-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 205753-10-2 HCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]glycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

PAGE 1-B

RN 318286-06-5 HCAPLUS

CN Acetamide, N-[O-(N-acetyl-4,7,8,9-tetra-O-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.3)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-.beta.-D-glucopyranosyl]-2-amino-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 318286-10-1 HCAPLUS

CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[(aminoacetyl)amino]phenyl]methy l]-, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 318286-61-2 HCAPLUS

CN Glycinamide, 4,4'-(1,4-butanediyl)bis[glycylglycylglycyl-, dihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A 
$$\begin{matrix} \text{O} & \text{O} & \text{O} & \text{O} \\ || & || & || & || \\ \text{H}_2\text{N}-\text{CH}_2-\text{C}-\text{NH}-\text{CH}_2-\text{C}-\text{NH}-\text{CH}_2-\text{C}-\text{NH}-\text{(CH}_2)}_4-\text{NH}-\text{C}- \end{matrix}$$

●2 HCl

PAGE 1-B

RN 318286-67-8 HCAPLUS

CN .beta.-D-Glucopyranoside, 3-aminopropyl O-(N-acetyl-4,7,8,9-tetra-O-acetyl-alpha.-neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 14302-75-1P 32564-25-3P 205753-09-9P 226408-84-0P 318285-90-4P 318285-93-7P 318285-95-9P 318286-08-7P 318286-16-7P 318286-19-0P 318286-21-4P 318286-23-6P 318286-25-8P 318286-27-0P 318286-29-2P 318286-31-6P 318286-33-8P 318286-35-0P 318286-37-2P 318286-41-8P 318286-43-0P 318286-57-6P 318286-59-8P 318286-69-0P 318510-95-1P 318511-00-1P 318511-08-9P 318511-10-3P 318511-11-4P 318511-17-0P 318511-35-2P 318511-41-0P 318511-44-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of self-assocg. compds. and their aggregate bodies for use as medicaments)

RN 14302-75-1 HCAPLUS

CN 1,3-Propanediamine, 2,2-bis(aminomethyl)-, tetrahydrochloride (8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2-\text{NH}_2 \\ | \\ \text{H}_2\text{N}-\text{CH}_2-\text{C}-\text{CH}_2-\text{NH}_2 \\ | \\ \text{CH}_2-\text{NH}_2 \end{array}$$

#### •4 HCl

RN 32564-25-3 HCAPLUS

CN Hexanedioic acid, bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)

RN 205753-09-9 HCAPLUS

CN 2,5,9,12-Tetraazatridecanedioic acid, 7,7-bis[[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]methyl]-4,10-dioxo-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 226408-84-0 HCAPLUS

CN Hexanoic acid, 6-[[3-[(3-O-.alpha.-D-galactopyranosyl-.beta.-D-galactopyranosyl)oxy]propyl]amino]-6-oxo-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 318285-90-4 HCAPLUS

CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[[[[6-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxohexyl]amino]acetyl]amino]phenyl]methyl ]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

∕OBu-t

RN 318285-93-7 HCAPLUS

CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[(20,20-dimethyl-1,4,11,18-tetraoxo-19-oxa-3,10,17-triazaheneicos-1-yl)amino]phenyl]methyl]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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## PAGE 1-B

CN

RN 318285-95-9 HCAPLUS

.alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[(27,27-dimethyl-1,4,11,18,25-pentaoxo-26-oxa-3,10,17,24-tetraazaoctacos-1-yl)amino]phenyl]methyl]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$(CH_2)$$
 5  $(CH_2)$  5  $N$  OBu-t

RN 318286-08-7 HCAPLUS

CN Hexanoic acid, 6-[[2-[[O-(N-acetyl-4,7,8,9-tetra-O-acetyl-.alpha.-neuraminosyl)-(1.fwdarw.3)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-.beta.-D-glucopyranosyl]amino]-2-oxoethyl]amino]-6-oxo-, 1-(4-nitrophenyl) ester (9CI) (CA INDEX NAME)

 ${\tt Absolute \ stereochemistry.}$ 

PAGE 1-A

PAGE 1-B

RN 318286-16-7 HCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]glycylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycyllon, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 1-C

RN 318286-19-0 HCAPLUS

CN Glycine, glycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine, tetrahydrochloride (9CI) (CA INDEX NAME)

#### •4 HCl

RN 318286-21-4 HCAPLUS

CN Glycine, glycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

RN 318286-23-6 HCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]glycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

PAGE 1-B

RN 318286-25-8 HCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]glycylglyc

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 1-D

— OBu−t

RN 318286-27-0 HCAPLUS

CN Glycine, N-(6-amino-1-oxohexyl)glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine, tetrahydrochloride (9CI) (CA INDEX NAME)

### ● 4 HCl

$$\begin{array}{c|c} & & R \\ | & \\ - & CH_2 - C - NH - CH_2 \\ | & \\ O \end{array}$$

PAGE 1-C

RN 318286-29-2 HCAPLUS

CN Glycine, N-(6-amino-1-oxohexyl)glycylglycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 1-C

RN 318286-31-6 HCAPLUS

CN Glycine, N-[6-[(6-amino-1-oxohexyl)amino]-1-oxohexyl]glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

## ● 4 HCl

PAGE 1-B

PAGE 1-C

RN 318286-33-8 HCAPLUS

CN Glycine, N-[6-[(6-amino-1-oxohexyl)amino]-1-oxohexyl]glycylglycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA

INDEX NAME)

$$-NH-CH_2-C-NH-CH_2-C-NH-CH_2$$

PAGE 1-C

RN 318286-35-0 HCAPLUS

CN Glycine, N-[6-[[6-[(6-amino-1-oxohexyl)amino]-1-oxohexyl]amino]-1-oxohexyl]glycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

#### ● 4 HC1

PAGE 1-B

$$\begin{array}{c|c} & & & & & R \\ || & & & | \\ - & \text{NH-} & \text{CH}_2 - \text{C-} & \text{NH-} & \text{CH}_2 - \text{C-} & \text{NH-} & \text{CH}_2 \\ || & & & || \\ & & & & O \end{array}$$

PAGE 1-C

PAGE 1-D

RN 318286-37-2 HCAPLUS

CN Glycine, N-[6-[[6-[(6-amino-1-oxohexyl)amino]-1-oxohexyl]amino]-1-oxohexyl]glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

PAGE 1-C

PAGE 1-D

RN 318286-41-8 HCAPLUS

CN .alpha.-Neuraminic acid, 2,2'-O-[[12,12-bis[[[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]amino]methyl]-1,4,9,15,20,23-hexaoxo-3,10,14,21-tetraazatricosane-1,23-diyl]bis(imino-4,1-phenylenemethylene)]bis[N-acetyl-, dimethyl ester, 4,4',7,7',8,8',9,9'-octaacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

RN 318286-43-0 HCAPLUS

.alpha.-Neuraminic acid, 2,2'-O-[[15,15-bis[[[[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]amino]acetyl]amino]methyl]
1,4,9,12,18,21,16,29-octaoxo-3,10,13,17,20,27-hexaazanonacosane-1,29-diyl]bis(imino-4,1-phenylenemethylene)]bis[N-acetyl-, dimethyl ester,4,4',7,7',8,8',9,9'-octaacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

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PAGE 2-A

PAGE 2-B

PAGE 2-C

RN 318286-57-6 HCAPLUS

CN Glycine, glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

● 4 HCl

PAGE 1-B

PAGE 1-C

-  $\mathrm{NH}_2$ 

RN 318286-59-8 HCAPLUS
CN Glycine, glycylglycylglycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

● 4 HCl

PAGE 1-B

PAGE 1-C

RN 318286-69-0 HCAPLUS

CN Hexanoic acid, 6-[[3-[[0-(N-acetyl-4,7,8,9-tetra-0-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.6)-0-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy-.beta.-D-glucopyranosyl]oxy]propyl]amino]-6-oxo-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 318510-95-1 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318511-00-1 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318511-08-9 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318511-10-3 HCAPLUS

CN Glycine, N-[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318511-11-4 HCAPLUS

CN Glycine, N-[6-[[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]amino]-1-oxohexyl]amino]-1-oxohexyl]glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 318511-17-0 HCAPLUS

CN Glycine, N-[30-[[4-[[(N-acetyl-4,7,8,9-tetra-0-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-1,8,15,22,27,30-hexaoxo-7,14,21,28-

tetraazatriacont-1-yl]glycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- RN 318511-35-2 HCAPLUS
- CN Glycine, N-[6-[[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-6-oxohexyl]amino]-1,6-dioxohexyl]glycylglycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- RN 318511-41-0 HCAPLUS
- CN Glycine, N-[6-[[6-[[2-[[4-[[(N-acetyl-4,7,8,9-tetra-0-acetyl-1-methyl-alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-6-oxohexyl]amino]-6-oxohexyl]amino]-1,6-dioxohexyl]glycylglycy
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- RN 318511-44-3 HCAPLUS
- CN Glycine, N-[30-[[4-[[(N-acetyl-4,7,8,9-tetra-O-acetyl-1-methyl-.alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-1,6,13,20,27,30-hexaoxo-7,14,21,28-tetraazatriacont-1-yl]glycylglycylglycylglycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)
- \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*
- IT 318285-97-1P 318285-99-3P 318286-01-0P 318286-03-2P 318286-45-2P 318286-63-4P
  - RL: SPN (Synthetic preparation); PREP (Preparation)
     (prepn. of self-assocg. compds. and their aggregate bodies for use as
     medicaments)
- RN 318285-97-1 HCAPLUS
- CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[[[[6-(4-nitrophenoxy)-1,6-dioxohexyl]amino]acetyl]amino]phenyl]methyl]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[[[6-[[6-(4-nitrophenoxy)-1,6-dioxohexyl]amino]-1-oxohexyl]amino]acetyl]amino]phenyl]methyl]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

vat.

## PAGE 1-B

RN 318286-01-0 HCAPLUS

CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[[[[6-[[6-[[6-(4-nitrophenoxy)-1,6-dioxohexyl]amino]-1-oxohexyl]amino]-1-oxohexyl]amino]acetyl]amino]phen yl]methyl]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CA INDEX NAME)

PAGE 1-B

RN 318286-03-2 HCAPLUS

CN .alpha.-Neuraminic acid, N-acetyl-2-O-[[4-[[30-(4-nitrophenoxy)-1,4,11,18,25,30-hexaoxo-3,10,17,24-tetraazatriacont-1-yl]amino]phenyl]methyl]-, methyl ester, 4,7,8,9-tetraacetate (9CI) (CIINDEX NAME)

PAGE 1-B

$$\begin{array}{c|c}
 & O \\
 & N \\
 & N \\
 & O
\end{array}$$

$$\begin{array}{c}
 & H \\
 & N \\
 & O
\end{array}$$

$$\begin{array}{c}
 & CH_2)_4 \\
 & O
\end{array}$$

$$\begin{array}{c}
 & O \\
 & NO_2
\end{array}$$

RN 318286-45-2 HCAPLUS

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CN .alpha.-Neuraminic acid, 2,2'-O-[[12,12-bis[[[6-[[2-[[4-[[(N-acetyl-alpha.-neuraminosyl)oxy]methyl]phenyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]amino]methyl]-1,4,9,15,20,23-hexaoxo-3,10,14,21-tetraazatricosane-1,23-diyl]bis(imino-4,1-phenylenemethylene)]bis[N-acetyl-(9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 2-B

RN 318286-63-4 HCAPLUS CN Glycinamide, 6,6'-(1,4-butanediyl)bis[glycylglycylglycylglycylglycylglycylglycylglycyl-,

dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

PAGE 1-C

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L41 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS
ΑN
    2000:117249 HCAPLUS
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DN 132:161232

Compounds, including saccharide compounds, for treatment of bacterial ΤI infections, and preparation thereof

IN Bundle, David R.; Kitov, Pavel; Read, Randy J.; Ling, Hong; Armstrong,

PA The Governors of the University of Alberta, Can.

SO PCT Int. Appl., 96 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM G01N033-53

CC 1-5 (Pharmacology)

Section cross-reference(s): 33, 63

FAN.CNT 3

	PATENT NO.				KIND		DATE			APPLICATION NO.					DATE				
PI	WO	2000008467			A2		2000	0217		WO 1999-CA725					19990806				
	WO	2000008467			A3		20000706												
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		PT, SE																	
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	ΑU				A1 B2		20000228 20021114			AU 1999-51450					19990806				
	ΑU																		
	EΡ				A2		20010530			EP 1999-936219				9	19990806				
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	FI															
PRAI	US	1998-130495 1999-317290			Α		1998	0807											
	US				Α		1999	0524											
	WO	1999-CA725			M		1999	0806											

Compds. which bind to toxins assocd. with enteric bacterial infection; AΒ compns. including the compds., methods for the neutralization of toxins in a patient, and methods for the diagnosis of bacterial and viral infections are disclosed. Toxins which can be bound by the compds. include pentameric toxins, for example SLTs (shiga-like toxins), such as those from Salmonella, Campylobacter and other bacteria, verotoxins from E. coli, cholera toxin, Clostridium difficile toxins A and B, bacterial pili from enteropathogenic E. coli and enterotoxigenic E. coli and viral lectins, such as viral hemagglutinins. The compds. include a core mol. bound to a plurality of linker arms, which in turn are bound to a plurality of bridging moieties, which in turn are bound to at least one, and preferably, two or more ligands which bind to the toxin. Examples of suitable ligands include di- and for trisaccharide moieties. The di- or tri-saccharide moieties themselves are active in binding to the SLTs. The presence of a plurality of bridged dimers of the ligands is responsible for the increased binding affinity of the compds. relative to the ligands themselves. In one embodiment, the compds., when administered in a timely fashion to a patient suffering from enteric E. coli infection, inhibit progression of this infection into hemolytic uremic syndrome (HUS).

ST antibacterial bacterial toxin saccharide deriv prepn; bacteria virus infection diagnosis; Escherichia hemolytic uremic syndrome saccharide deriv

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(B, Clostridium difficile; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(Shiga-like toxin I; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(Shiga-like toxin II; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(Shiga-like toxin; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Carbohydrates, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (aldaric acids; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Peptides, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (amino acids; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Infection

(bacterial, diagnosis; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(cholera; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Antibacterial agents

Campylobacter

Drug delivery systems

Salmonella

(compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Agglutinins and Lectins

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Amino acids, biological studies
Disaccharides

Monosaccharides

Oligosaccharides, biological studies

Trisaccharides

RL: BSU (Biological study, unclassified); BIOL (Biological study) (compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Escherichia coli

(enterotoxigenic; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Pilus

(from enteropathogenic E. coli; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Drug delivery systems

(injections; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Fluorescent substances

(label; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Enzymes, biological studies

Radionuclides, biological studies

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (label; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Drug delivery systems

(oral; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Intestinal bacteria

(pathogenic, pili from enteropathogenic E. coli; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Escherichia coli

(pili from enteropathogenic E. coli; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Alcohols, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (polyhydric; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Albumins, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(saccharide derivs.; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Toxins

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(toxin A, Clostridium difficile; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Clostridium difficile

(toxins A and B; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT Virus

(viral lectin; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

IT 258873-66-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

TT 79-06-1D, Acrylamide, derivs. 574-93-6D, Phthalocyanine,
derivs. 12619-70-4D, Cyclodextrin, derivs. 13117-26-5D
, derivs. 54832-51-8D, derivs. 66580-68-5D, derivs.

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
        (compds., including saccharide compds., for treatment of bacterial
       infections, and prepn. thereof)
    58-85-5 9013-20-1, Streptavidin
    RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (label; compds., including saccharide compds., for treatment of
       bacterial infections, and prepn. thereof)
    244076-91-3P 244076-92-4P 244076-93-5P
    244076-96-8P 244076-97-9P 244076-98-0P
    .244076-99-1P 244077-00-7P 244077-01-8P
    244077-02-9P 244077-03-0P 244077-04-1P
    244077-05-2P 244077-06-3P 244077-07-4P
    244077-08-5P 244077-09-6P 258857-10-2P
    258857-11-3P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reaction; compds., including saccharide compds., for
       treatment of bacterial infections, and prepn. thereof)
    98-88-4, Benzoyl chloride 100-39-0 106-95-6,
    Allyl bromide, reactions 107-15-3, 1,2-Ethanediamine, reactions
    373-44-4, 1,8-Diaminooctane 616-29-5,
    1,3-Diamino-2-hydroxypropane 1125-88-8, .alpha.,.alpha.-
    Dimethoxytoluene 2365-48-2, Methyl thioglycolate
    5231-87-8 7693-46-1, 4-Nitrophenyl chloroformate
    41110-63-8 63976-06-7 102674-58-8
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction; compds., including saccharide compds., for treatment of
       bacterial infections, and prepn. thereof)
    258873-66-4P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (compds., including saccharide compds., for treatment of bacterial
       infections, and prepn. thereof)
    258873-66-4 HCAPLUS
    Carbamic acid, [.beta.-D-glucopyranose-1,2,3,4,6-penta-O-ylpentakis[3,1-
    propanediylthio(1-oxo-2,1-ethanediyl)imino-2,1-ethanediylimino(3,4-dioxo-1-
    cyclobutene-2,1-diyl)imino-8,1-octanediyliminocarbonyloxy-3,1,2-
    propanetriyl]]decakis-, decaester with methyl O-.alpha.-D-galactopyranosyl-
     (1.fwdarw.4)-O-2-O-(2-hydroxyethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-
     .beta.-D-glucopyranoside (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
    79-06-1D, Acrylamide, derivs. 574-93-6D, Phthalocyanine,
    derivs. 12619-70-4D, Cyclodextrin, derivs. 13117-26-5D
     , derivs. 54832-51-8D, derivs. 66580-68-5D, derivs.
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
        (compds., including saccharide compds., for treatment of bacterial
       infections, and prepn. thereof)
    79-06-1 HCAPLUS
    2-Propenamide (9CI) (CA INDEX NAME)
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CN 29H, 31H-Phthalocyanine (9CI) (CA INDEX NAME)

RN 12619-70-4 HCAPLUS

CN Cyclodextrin (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 13117-26-5 HCAPLUS

CN D-Galactose, 4-O-.alpha.-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 54832-51-8 HCAPLUS

CN D-Glucose, O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 66580-68-5 HCAPLUS

CN D-Glucose, O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

58-85-5 9013-20-1, Streptavidin IT

> RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (label; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

58-85-5 HCAPLUS RN

CN . 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS, 4S, 6aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 9013-20-1 HCAPLUS

Streptavidin (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 244076-91-3P 244076-92-4P 244076-93-5P

244076-96-8P 244076-97-9P 244076-98-0P

244076-99-1P 244077-00-7P 244077-01-8P

244077-02-9P 244077-03-0P 244077-04-1P

244077-05-2P 244077-06-3P 244077-07-4P

244077-08-5P 244077-09-6P 258857-10-2P

258857-11-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)

RN244076-91-3 HCAPLUS

CN D-Glucopyranose, 4-O-(3,4,6-tri-O-acetyl-2-O-2-propenyl-.beta.-Dgalactopyranosyl)-, tetraacetate (9CI) (CA INDEX NAME)

RN 244076-92-4 HCAPLUS

CN .alpha.-D-Glucopyranosyl chloride, 4-O-(3,4,6-tri-O-acetyl-2-O-2-propenyl-beta.-D-galactopyranosyl)-, triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-93-5 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-(2-O-2-propenyl-.beta.-D-galactopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 244076-96-8 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 2,3,6-tris-O-(phenylmethyl)-4-O-[3-O-(phenylmethyl)-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-97-9 HCAPLUS

Absolute stereochemistry. Rotation (+).

RN 244076-98-0 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-6-O-benzoyl-3-O-(phenylmethyl)-2O-2-propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244076-99-1 HCAPLUS

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CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3-O-(phenylmethyl)-2-O-2propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-00-7 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-2-O-2propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-01-8 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-(2-hydroxyethyl)-3,6-bis-O(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-02-9 HCAPLUS

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CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-[2-[(4-nitrophenoxy)carbonyl]oxy]ethyl]-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A

PAGE 2-A

RN 244077-03-0 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[(2-hydroxy-1,3-propanediyl)bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A

PAGE 1-B

PAGE 2-A

PAGE 2-B

RN 244077-04-1 HCAPLUS

.beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[(4-nitrophenoxy)carbonyl]oxy]1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl
O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-B

PAGE 2-A

PAGE 2-B

RN 244077-05-2 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[(8-aminooctyl)amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A

PAGE 2-A

PAGE 2-B

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PAGE 3-B

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RN 244077-06-3 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[(8-aminooctyl)amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-B

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PAGE 2-B

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RN 244077-07-4 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[[8-[(2-ethoxy-3,4-dioxo-1-cyclobuten-1-yl)amino]octyl]amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A

PAGE 2-B

RN 244077-08-5 HCAPLUS

CN Acetic acid, [[3-[[2,3,4,6-tetrakis-O-[3-[(2-methoxy-2-oxoethyl)thio]propyl]-.beta.-D-glucopyranosyl]oxy]propyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244077-09-6 HCAPLUS

CN Acetamide, N-(2-aminoethyl)-2-[[3-[[2,3,4,6-tetrakis-0-[3-[[2-[(2-aminoethyl)amino]-2-oxoethyl]thio]propyl]-.beta.-D-glucopyranosyl]oxy]propyl]thio]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 258857-10-2 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-[4,6-O-(phenylmethylene)-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 258857-11-3 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 2,3,6-tris-O-(phenylmethyl)-4-O-[3-O-(phenylmethyl)-4,6-O-(phenylmethylene)-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

IT 98-88-4, Benzoyl chloride 100-39-0 106-95-6,
 Allyl bromide, reactions 107-15-3, 1,2-Ethanediamine, reactions
373-44-4, 1,8-Diaminooctane 616-29-5,
 1,3-Diamino-2-hydroxypropane 1125-88-8, .alpha.,.alpha. Dimethoxytoluene 2365-48-2, Methyl thioglycolate
 5231-87-8 7693-46-1, 4-Nitrophenyl chloroformate
 4110-63-8 63976-06-7 102674-58-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction; compds., including saccharide compds., for treatment of bacterial infections, and prepn. thereof)
RN 98-88-4 HCAPLUS
CN Benzoyl chloride (8CI, 9CI) (CA INDEX NAME)

RN 100-39-0 HCAPLUS CN Benzene, (bromomethyl)- (9CI) (CA INDEX NAME)

Ph-CH2-Br

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RN 106-95-6 HCAPLUS CN 1-Propene, 3-bromo- (9CI) (CA INDEX NAME)

 $Br-CH_2-CH-CH_2$ 

RN 107-15-3 HCAPLUS CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

RN 373-44-4 HCAPLUS .
CN 1,8-Octanediamine (6CI, 8CI, 9CI) (CA INDEX NAME)

 $H_2N-(CH_2)_8-NH_2$ 

RN 616-29-5 HCAPLUS

CN 2-Propanol, 1,3-diamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ | \\ \text{H}_{2}\text{N-CH}_{2}\text{-CH-CH}_{2}\text{-NH}_{2} \end{array}$$

RN 1125-88-8 HCAPLUS

CN Benzene, (dimethoxymethyl) - (9CI) (CA INDEX NAME)

RN 2365-48-2 HCAPLUS

CN Acetic acid, mercapto-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 5231-87-8 HCAPLUS

CN 3-Cyclobutene-1,2-dione, 3,4-diethoxy- (9CI) (CA INDEX NAME)

RN 7693-46-1 HCAPLUS

CN Carbonochloridic acid, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

RN 41110-63-8 HCAPLUS

CN .alpha.-D-Galactopyranosyl chloride, 2,3,4,6-tetrakis-O-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 63976-06-7 HCAPLUS

CN .beta.-D-Glucopyranoside, 2-propenyl 2,3,4,6-tetra-O-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 102674-58-8 HCAPLUS

CN D-Glucose, 4-O-[6-O-(1-methoxy-1-methylethyl)-3,4-O-(1-methylethylidene)-.beta.-D-galactopyranosyl]-2,3:5,6-bis-O-(1-methylethylidene)-, dimethyl acetal (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L41 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS

AN 1999:635458 HCAPLUS

DN 131:228948

TI Preparation of dendrimer oligosaccharides for treatment of bacterial dysentery

IN Bundle, David R.; Kitov, Pavel; Read, Randy J.; Ling, Hong; Armstrong, Glen

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     The Governors of the University of Alberta, Can.
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     U.S., 27 pp.
     CODEN: USXXAM
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     ICM A61K031-70
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     33-4 (Carbohydrates)
     Section cross-reference(s): 1, 10, 63
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                                                           19990806
           AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI
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PRAI US 1998-130495
     US 1999-317290
                            19990524
                      Α
     WO 1999-CA725
                      W
                           19990806
AB
     Compds. which bind to shiga-like toxins (SLT) assocd. with enteric E. coli
     infection, compns. including the compds., methods for the neutralization
     of (SLT) in a patient, and methods for the diagnosis of enteric E. coli
     infection are disclosed. The compds. MFC-(LA)n-(BM)n were prepd. as
     shiga-like toxins wherein; MFC is a multifunctional core mol., LA is a
     linker arm, BM is a bridging mol. which includes two or more di- or
     trisaccharides, and which can optionally include large oligosaccharides, n
     is, independently, between 3 and 20, the di- or trisaccharide moiety are
     optionally linked to between one and eight addnl. saccharide moieties, and
     include an individual saccharide moiety selected from the group consisting
     of .alpha.Gal(1-4).beta.Gal, .alpha.Gal(1-4).beta.Gal(1-4).beta.GlcNAc,
     and .alpha.Gal(1-4).beta.Gal(1-4).beta.Glc, the bridging moieties are
     bound to at least one linker arm, the linker arms are, independently,
     C6-20 straight, branched or cyclic alkanes, in which one or more of the
     carbons may optionally be replaced with an O, S, or amine, and the linker
     arms can optionally be functionalized at one or more positions with a
     functional group selected from the group consisting of aryl, substituted
     aryl, heteroaryl, substituted heteroaryl, heterocyclic and substituted
     heterocyclic. The di- or tri-saccharide moieties themselves are active in
     binding to the SLTs. The presence of a plurality of bridged dimers of the
     di- and tri-saccharides is responsible for the increased binding affinity
     of the compds. relative to the di- and tri-saccharides themselves. The
     compds., when administered in a timely fashion to a patient suffering from
     enteric E. coli infection, inhibit progression of this infection into
     hemolytic uremic syndrome (HUS).
     hemolytic uremic syndrome inhibitor dendrimer oligosaccharide prepn; shiga
ST
     like toxin bactericide E coli oligosaccharide prepn; dendrimer
     oligosaccharide prepn cytotoxicity antibacterial
ΙT
     Toxins
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (Shiga-like toxin; prepn. of dendrimer oligosaccharides for treatment
```

of bacterial dysentery)

```
IT
     Kidney, disease
        (hemolytic-uremic syndrome; prepn. of dendrimer oligosaccharides for
        treatment of bacterial dysentery)
ΙT
     Antibacterial agents
     Cytotoxicity
     Dysentery
     Escherichia coli
        (prepn. of dendrimer oligosaccharides for treatment of bacterial
        dysentery)
     Dendritic polymers
ΙT
     Oligosaccharides, preparation
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of dendrimer oligosaccharides for treatment of bacterial
        dysentery)
     244077-03-0P 244077-07-4P 244094-61-9P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of dendrimer oligosaccharides for treatment of bacterial
        dysentery)
IT
     373-44-4, 1,8-Diaminooctane 492-61-5,
     .beta.-D-Glucopyranose 616-29-5, 1,3-Diamino-2-hydroxypropane
     5231-87-8 7693-46-1, 4-Nitrophenyl chloroformate
     41110-63-8 244076-90-2 244077-04-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of dendrimer oligosaccharides for treatment of bacterial
        dysentery)
IT
     63976-06-7P 244076-91-3P 244076-92-4P
     244076-93-5P 244076-94-6P 244076-95-7P
     244076-96-8P 244076-97-9P 244076-98-0P
     244076-99-1P 244077-00-7P 244077-01-8P
     244077-02-9P 244077-05-2P 244077-06-3P
     244077-08-5P 244077-09-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of dendrimer oligosaccharides for treatment of bacterial
        dysentery)
RE.CNT
        30
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- IT 244077-03-0P 244077-07-4P 244094-61-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of dendrimer oligosaccharides for treatment of bacterial dysentery)

RN 244077-03-0 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[(2-hydroxy-1,3-propanediyl)bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

R S S Ph Ph O

PAGE 1-A

PAGE 1-B

PAGE 2-A Ph

PAGE 2-B

RN 244077-07-4 HCAPLUS .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[[8-[(2-ethoxy-3,4-dioxo-1-cyclobuten-1-yl)amino]octyl]amino]carbonyl]oxy]-1,3-CN

propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-

(1.fwdarw.4) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$\begin{array}{ccc} / & & \bigvee \\ \text{EtO} & & \overset{N}{\text{H}} \end{array}$$

PAGE 2-B

RN 244094-61-9 HCAPLUS

.beta.-D-Glucopyranoside, methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-(2-hydroxyethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-, decaester with [2-[[[8-[[3,4-dioxo-2-[[2-[[[2-[[2-[[2-[[2-[[2-[[2-[[8-[[2-([2-[[2-[[2-[[2-[[3,4,6-tetrakis-O-[2-[[2-[[2-[[8-[[2-(carboxyamino)-1-(carboxyamino)methyl]ethoxy]carbonyl]amino]octyl]amino]-3,4-dioxo-1-cyclobuten-1-yl]amino]ethyl]amino]-2-oxoethyl]thio]ethyl]-.beta.-D-glucopyranosyl]oxy]ethyl]thio]acetyl]amino]ethyl]amino]-1-cyclobuten-1-yl]amino]octyl]amino]carbonyl]oxy]-1,3-propanediyl]bis[carbamic acid] (9CI) (CA INDEX NAME)

CN 1,8-Octanediamine (6CI, 8CI, 9CI) (CA INDEX NAME)

 $H_2N-(CH_2)_8-NH_2$ 

RN 492-61-5 HCAPLUS CN .beta.-D-Glucopyranose (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 616-29-5 HCAPLUS

CN 2-Propanol, 1,3-diamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ | \\ \text{H}_{2}\text{N}-\text{CH}_{2}-\text{CH}-\text{CH}_{2}-\text{NH}_{2} \end{array}$$

RN 5231-87-8 HCAPLUS

CN 3-Cyclobutene-1,2-dione, 3,4-diethoxy- (9CI) (CA INDEX NAME)

RN 7693-46-1 HCAPLUS

CN Carbonochloridic acid, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

RN 41110-63-8 HCAPLUS

CN .alpha.-D-Galactopyranosyl chloride, 2,3,4,6-tetrakis-O-(phenylmethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244076-90-2 HCAPLUS

CN D-Glucose, 4-O-[6-O-(1-methoxy-1-methylethyl)-3,4-O-(1-methylethylidene)-.beta.-D-galactopyranosyl]-2,3:5,6-bis-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244077-04-1 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[(4-nitrophenoxy)carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-B

O Ph

PAGE 2-A

Ph. O

PAGE 2-B

Absolute stereochemistry.

$$H_2C$$
 $O$ 
 $R$ 
 $R$ 
 $O$ 
 $CH_2$ 

RN 244076-91-3 HCAPLUS

CN D-Glucopyranose, 4-0-(3,4,6-tri-O-acetyl-2-O-2-propenyl-.beta.-D-galactopyranosyl)-, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244076-92-4 HCAPLUS

CN .alpha.-D-Glucopyranosyl chloride, 4-O-(3,4,6-tri-O-acetyl-2-O-2-propenyl-beta.-D-galactopyranosyl)-, triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-93-5 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-(2-O-2-propenyl-.beta.-D-galactopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 244076-94-6 HCAPLUS

=

CN .beta.-D-Glucopyranoside, methyl 4-O-[4,6-O-[(S)-phenylmethylene]-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 244076-95-7 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 2,3,6-tris-O-(phenylmethyl)-4-O-[3-O-(phenylmethyl)-4,6-O-[(S)-phenylmethylene]-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-96-8 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 2,3,6-tris-O-(phenylmethyl)-4-O-[3-O-(phenylmethyl)-2-O-2-propenyl-.beta.-D-galactopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-97-9 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl 4-O-[6-O-benzoyl-3-O-(phenylmethyl)-2-O-2-propenyl-.beta.-D-galactopyranosyl]-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244076-98-0 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-6-O-benzoyl-3-O-(phenylmethyl)-2O-2-propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244076-99-1 HCAPLUS

ش

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3-O-(phenylmethyl)-2-O-2propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-00-7 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-2-O-2propenyl-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-01-8 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-(2-hydroxyethyl)-3,6-bis-O(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 244077-02-9 HCAPLUS

CN .beta.-D-Glucopyranoside, methyl O-2,3,4,6-tetrakis-O-(phenylmethyl).alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-2-O-[2-[[(4nitrophenoxy)carbonyl]oxy]ethyl]-3,6-bis-O-(phenylmethyl)-.beta.-Dgalactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 2-A

RN 244077-05-2 HCAPLUS

.beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[(8-aminooctyl)amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-2,3,4,6-tetrakis-O-(phenylmethyl)-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-3,6-bis-O-(phenylmethyl)-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2,3,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

z. .

PAGE 1-A

PAGE 2-A

PAGE 2-B

....OMe

Ph

PAGE 3-B

Ph

RN 244077-06-3 HCAPLUS

CN .beta.-D-Glucopyranoside, 2',2''''-O-[[2-[[[(8-aminooctyl)amino]carbonyl]oxy]-1,3-propanediyl]bis(iminocarbonyloxy-2,1-ethanediyl)]bis[methyl O-.alpha.-D-galactopyranosyl-(1.fwdarw.4)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

## PAGE 1-A

## PAGE 1-B

PAGE 2-B

но

RN 244077-08-5 HCAPLUS

CN Acetic acid, [[3-[[2,3,4,6-tetrakis-O-[3-[(2-methoxy-2-oxoethyl)thio]propyl]-.beta.-D-glucopyranosyl]oxy]propyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244077-09-6 HCAPLUS

CN Acetamide, N-(2-aminoethyl)-2-[[3-[[2,3,4,6-tetrakis-O-[3-[[2-[(2-aminoethyl)amino]-2-oxoethyl]thio]propyl]-.beta.-D-glucopyranosyl]oxy]propyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

NH<sub>2</sub>

NH2

ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2003 ACS ΑN 1999:238153 HCAPLUS DN 131:19206 TI Synthesis of neoglycoconjugate dendrimers ΑU Tsvetkov, Dmitry E.; Cheshev, Pavel E.; Tuzikov, Alexander B.; Pazynina, Galina V.; Bovin, Nikolai V.; Rieben, Robert; Nifant'ev, Nikolay E. N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, CS Moscow, 117913, Russia SO Mendeleev Communications (1999), (2), 47-50 CODEN: MENCEX; ISSN: 0959-9436 PB Russian Academy of Sciences DT Journal LA English CC 33-4 (Carbohydrates) Section cross-reference(s): 15 A series of polydentate dendritic neoglycoconjugates which contain 4, 8, AB 16, 32 B-disaccharide ligands were designed as probes to assess the influence of inter-ligand distance on binding to anti-B-disaccharide Igs. structure activity binding Ig neoglycoconjugate dendrimer synthesis; ST neoglycoconjugate dendrimer synthesis disaccharide binding Ig ΙT Polyamines Polyamines Polyamines RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (polyamide-, dendrimers; synthesis of neoglycoconjugate dendrimers and the influence of inter-ligand distance on binding to anti-B-disaccharide Igs) ΙT Dendritic polymers RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (polyamide-polyamines; synthesis of neoglycoconjugate dendrimers and the influence of inter-ligand distance on binding to anti-B-disaccharide Igs) IT Polyamides, preparation Polyamides, preparation Polyamides, preparation

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(polyamine-, dendrimers; synthesis of neoglycoconjugate dendrimers and the influence of inter-ligand distance on binding to anti-B-disaccharide Igs)

IT Structure-activity relationship

(synthesis of neoglycoconjugate dendrimers and the influence of

```
inter-ligand distance on binding to anti-B-disaccharide Igs)
IT
     Disaccharides
     Glycoconjugates
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (synthesis of neoglycoconjugate dendrimers and the influence of
        inter-ligand distance on binding to anti-B-disaccharide Igs)
ΙT
     Immunoglobulins
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (synthesis of neoglycoconjugate dendrimers and the influence of
        inter-ligand distance on binding to anti-B-disaccharide Igs)
ΙT
     26937-01-9DP, PAMAM, .alpha.-D-Gal(1.fwdarw.3)-.beta.-D-Gal
     terminated 26937-01-9P, PAMAM
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (dendritic; synthesis of neoglycoconjugate dendrimers and the influence
        of inter-ligand distance on binding to anti-B-disaccharide Igs)
ΙT
     96-33-3, Methyl acrylate 107-15-3, 1,2-Ethanediamine,
     reactions 124-09-4, 1,6-Hexanediamine, reactions
     32564-25-3 201667-63-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of neoglycoconjugate dendrimers and the influence of
        inter-ligand distance on binding to anti-B-disaccharide Igs)
TΤ
     194867-28-2P 226408-71-5P 226408-74-8P
     226408-77-1P 226408-79-3P 226408-80-6P
     226408-84-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis of neoglycoconjugate dendrimers and the influence of
        inter-ligand distance on binding to anti-B-disaccharide Igs)
IT
     226408-73-7P 226408-81-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of neoglycoconjugate dendrimers and the influence of
        inter-ligand distance on binding to anti-B-disaccharide Igs)
RE.CNT
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26937-01-9DP, PAMAM, .alpha.-D-Gal(1.fwdarw.3)-.beta.-D-Gal

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terminated 26937-01-9P, PAMAM
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (dendritic; synthesis of neoglycoconjugate dendrimers and the influence
        of inter-ligand distance on binding to anti-B-disaccharide Igs)
RN
     26937-01-9 HCAPLUS
CN
     2-Propenoic acid, methyl ester, polymer with 1,2-ethanediamine (9CI)
                                                                            (CA
     INDEX NAME)
     CM
          1
         107-15-3
     CRN
     CMF C2 H8 N2
H_2N-CH_2-CH_2-NH_2
          2
     CM
     CRN
         96-33-3
     CMF C4 H6 O2
MeO-C-CH=CH2
RN
     26937-01-9 HCAPLUS
     2-Propenoic acid, methyl ester, polymer with 1,2-ethanediamine (9CI) (CA
CN
     INDEX NAME)
     CM
          1
     CRN 107-15-3
     CMF C2 H8 N2
H2N-CH2-CH2-NH2
     CM
          2
     CRN 96-33-3
     CMF C4 H6 O2
MeO-C-CH-CH2
IT
     96-33-3, Methyl acrylate 107-15-3, 1,2-Ethanediamine,
     reactions 124-09-4, 1,6-Hexanediamine, reactions
     32564-25-3 201667-63-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of neoglycoconjugate dendrimers and the influence of
        inter-ligand distance on binding to anti-B-disaccharide Igs)
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96-33-3 HCAPLUS

RN

CN 2-Propenoic acid, methyl ester (9CI) (CA INDEX NAME)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

RN 124-09-4 HCAPLUS

CN 1,6-Hexanediamine (7CI, 8CI, 9CI) (CA INDEX NAME)

 $H_2N-(CH_2)_6-NH_2$ 

RN 32564-25-3 HCAPLUS

CN Hexanedioic acid, bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)

RN 201667-63-2 HCAPLUS

CN .beta.-D-Galactopyranoside, 3-aminopropyl 3-O-.alpha.-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 194867-28-2P 226408-71-5P 226408-74-8P 226408-77-1P 226408-79-3P 226408-80-6P

226408-84-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of neoglycoconjugate dendrimers and the influence of inter-ligand distance on binding to anti-B-disaccharide Igs)

RN 194867-28-2 HCAPLUS

# Z

CN .beta.-Alanine, N,N'-1,6-hexanediylbis[N-(3-methoxy-3-oxopropy1)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 226408-71-5 HCAPLUS
CN Propanamide, 3,3',3'',3'''-(1,6-hexanediyldinitrilo)tetrakis[N-(2-aminoethyl)- (9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 1-A

- ин2

RN 226408-74-8 HCAPLUS
CN 4,7,11,18,22,25-Hexaazaoctacosanedioic acid, 11,18-bis[3-[[2-[bis(3-methoxy-3-oxopropyl)amino]ethyl]amino]-3-oxopropyl]-4,25-bis(3-methoxy-3-oxopropyl)-8,21-dioxo-, dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-B

RN 226408-77-1 HCAPLUS

CN 4,7,11,18,22,25-Hexaazaoctacosanediamide, N,N'-bis(2-aminoethyl)-4,25-bis[3-[(2-aminoethyl)amino]-3-oxopropyl]-11,18-bis[3-[(2-[bis[3-[(2-aminoethyl)amino]-3-oxopropyl]amino]ethyl]amino]-3-oxopropyl]-8,21-dioxo-(9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} O \\ H_2N-CH_2-CH_2-NH-C-CH_2-CH_2 \\ H_2N-CH_2-CH_2-NH-C-CH_2-CH_2-N-CH_2-CH_2-NH-C-CH_2-CH_2-N \\ \\ O \\ \end{array}$$

PAGE 1-B

PAGE 2-B

RN 226408-79-3 HCAPLUS

CN 4,7,11,14,18,25,29,32,36,39-Decaazadotetracontanedioic acid,
11,32-bis[3-[[2-[bis(3-methoxy-3-oxopropyl)amino]ethyl]amino]-3-oxopropyl]18,25-bis[7-[3-[[2-[bis(3-methoxy-3-oxopropyl)amino]ethyl]amino]-3oxopropyl]-14-(3-methoxy-3-oxopropyl)-3,10,17-trioxo-18-oxa-4,7,11triazanonadec-1-yl]-4,39-bis(3-methoxy-3-oxopropyl)-8,15,28,35-tetraoxo-,
dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 2-A

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{R2-CH}_2\text{--CH}_2\text{--C-OMe} \end{array}$$

$$\begin{array}{c} \text{O} \\ || \\ \text{R4-CH}_2\text{--CH}_2\text{--C-OMe} \end{array}$$

PAGE 3-A

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{C-OMe} \\ \text{R5-CH}_2-\text{CH}_2-\text{C-NH-CH}_2-\text{CH}_2-\text{N-----} \text{R2} \\ || \\ \text{O} \end{array}$$

PAGE 3-B

PAGE 4-A

PAGE 4-B

$$\begin{array}{c} \text{O} \\ || \\ \text{CH}_2-\text{CH}_2-\text{C-OMe} \\ | \\ --\text{CH}_2-\text{N-CH}_2-\text{CH}_2-\text{C-OMe} \\ || \\ \text{O} \end{array}$$

RN 226408-80-6 HCAPLUS

CN 4,7,11,14,18,25,29,32,36,39-Decaazadotetracontanediamide,
18,25-bis[20-amino-14-[3-[(2-aminoethyl)amino]-3-oxopropyl]-7-[3-[[2-[bis[3-[(2-aminoethyl)amino]-3-oxopropyl]amino]ethyl]amino]-3-oxopropyl]3,10,17-trioxo-4,7,11,14,18-pentaazaeicos-1-yl]-N,N'-bis(2-aminoethyl)4,39-bis[3-[(2-aminoethyl)amino]-3-oxopropyl]-10,32-bis[3-[[2-[bis[3-[(2-aminoethyl)amino]-3-oxopropyl]amino]ethyl]amino]-3-oxopropyl]-8,15,28,35tetraoxo-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

æ.

PAGE 1-C

NH2

PAGE 2-C

RN 226408-84-0 HCAPLUS

CN Hexanoic acid, 6-[[3-[(3-O-.alpha.-D-galactopyranosyl-.beta.-D-galactopyranosyl)oxy]propyl]amino]-6-oxo-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## IT 226408-73-7P 226408-81-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of neoglycoconjugate dendrimers and the influence of inter-ligand distance on binding to anti-B-disaccharide Igs)

RN 226408-73-7 HCAPLUS

r.

CN 7,10,14,21,25,28-Hexaazatetratriacontanediamide, N,N'-bis[3-[(3-O-.alpha.-D-galactopyranosyl-.beta.-D-galactopyranosyl)oxy]propyl]-14,21-bis[3-[[2-[[6-[[3-[(3-O-.alpha.-D-galactopyranosyl-.beta.-D-galactopyranosyl)oxy]propyl]amino]-1,6-dioxohexyl]amino]ethyl]amino]-3-oxopropyl]-6,11,24,29-tetraoxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$\begin{array}{c|c}
R \\
N \\
N \\
H
\end{array}$$

$$\begin{array}{c}
H \\
N \\
H
\end{array}$$

$$\begin{array}{c}
(CH_2)_4 \\
N \\
H
\end{array}$$

$$\begin{array}{c}
(CH_2)_3 \\
O
\end{array}$$

PAGE 1-C

PAGE 2-B

RN 226408-81-7 HCAPLUS

CN Hexanediamide, N,N''-1,6-hexanediylbis[N'-[3-[(3-O-.alpha.-D-galactopyranosyl-.beta.-D-galactopyranosyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

OH OH OH OH 
$$(CH_2)_A$$
  $(CH_2)_B$   $(CH_2)_B$ 

L41 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:219739 HCAPLUS

DN 128:278972

ت:

TI Glycoconjugates as virus cell adhesion inhibitors

IN Bovin, Nikolai; Matrosovich, Mikhail; Tuzikov, Alexandr

```
; Chinarev, Alexandr; Gambaryan, Alexandra; Robertson, James
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PA Syntesome Gesellschaft fuer Med. Biochemie m.b.H., Germany; Bovin, Nikolai; Matrosovich, Mikhail; Tuzikov, Alexandr; Chinarev, Alexandr; Gambaryan, Alexandra; Robertson, James

SO PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DT Patent

LA German

IC ICM A61K047-48

CC 1-5 (Pharmacology)

Section cross-reference(s): 33

FAN.CNT 1

FAN.	PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
PI	WO 9814215		19980409		WO 1997-EP5389	19971001
	WO 9814215	A3	19980820			
•	W: CA, JP, U	IS				
	RW: AT, BE, C	H, DE,	DK, ES,	FI,	FR, GB, GR, IE, IT,	LU, MC, NL, PT, SE
	DE 19640791	A1	19980416		DE 1996-19640791	19961002
	EP 863769	A1·	19980916		EP 1997-948758	19971001
	EP 863769	B1	20020703			
	R: AT, BE, C	H, DE,	FR, GB,	IT,	LI	
	JP 2002514186	T2	20020514		JP 1998-516240	19971001
	AT 219947	E	20020715		AT 1997-948758	19971001
PRAI	DE 1996-19640791	A	19961002			
	WO 1997-EP5389	W	19971001			
os	MARPAT 128:278972	?			•	•
GI						

The host-cell adhesion by human influenza viruses is inhibited by 6'-sialyl-N-acetyllactosamine conjugates [I; R1, R3 = acyl, thioacyl; R2 = H, OH, ZA; A = (substituted) alkyl, (substituted) aryl; Z = O, S, NH; R4 = H, acyl; X = O, S, C1-4 alkylene; W = bifunctional spacer; P = multivalent carrier [polyacrylate, (N-substituted) polyacrylamide, (N-substituted) methacrylamide, poly(acrylic acid), polycarbonate, polyester, polyamide, polyanhydride, polyiminocarbonate, poly(ortho ester), polydioxanone, polyphosphazene, poly(hydroxy carboxylic acid), poly(amino acid), polysaccharide, protein, dextran, chitosan, glucan, liposomes, microparticles]]. I can bind to human influenza A (H1 and H3) and B viruses which have not been adapted by culturing in chicken eggs and therefore have an unaltered structure of the receptor-binding site on the

Ι

viral hemagglutinin; they are useful prophylactically and therapeutically against influenza virus infections. Thus, 6'-sialyl-N-acetyllactosamine ammonium salt was converted to its N-glycyl deriv. (II) by reaction with chloroacetic anhydride. Poly(4-nitrophenyl acrylate) was 20% substituted with II by reaction with II and ethanolamine to form II-substituted poly[N-(2-hydroxyethyl)acrylamide]. The affinity const. of this polymer conjugate for all strains of influenza A and B virus tested was in the range 0.01-0.1 .mu.M, as detd. by its inhibition of viral binding to fetuin.

ST virus cell adhesion inhibitor sialylacetyllactosamine deriv

IT Cell adhesion

(by viruses; glycoconjugates as virus cell adhesion inhibitors)

IT Liposomes

Microparticles

(conjugates with sialylacetyllactosamine; glycoconjugates as virus cell adhesion inhibitors)

IT Polyamides, biological studies

Polyanhydrides

Polycarbonates, biological studies

Polyesters, biological studies

Polyphosphazenes

Polysaccharides, biological studies

Proteins, general, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(conjugates with sialylacetyllactosamine; glycoconjugates as virus cell adhesion inhibitors)

IT Animal virus

Antiviral agents

Influenza virus

(glycoconjugates as virus cell adhesion inhibitors)

IT Glycoconjugates

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(glycoconjugates as virus cell adhesion inhibitors)

IT Carboxylic acids, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(hydroxy, polymers, conjugates with sialylacetyllactosamine; glycoconjugates as virus cell adhesion inhibitors)

IT Hemagglutinins

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(of influenza virus, binding of; glycoconjugates as virus cell adhesion inhibitors)

IT Esters, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(ortho acid, polymers, conjugates with sialylacetyllactosamine; glycoconjugates as virus cell adhesion inhibitors)

IT Polyamides, biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(poly(amino acids), conjugates with sialylacetyllactosamine;
glycoconjugates as virus cell adhesion inhibitors)

IT Receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

```
(virus binding to, inhibition of; glycoconjugates as virus cell
        adhesion inhibitors)
     78969-47-8, 6'-Sialyl-N-acetyllactosamine
ΙT
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (carrier conjugates; glycoconjugates as virus cell adhesion inhibitors)
IT
     31621-87-1, Polydioxanone
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (conjugates with sialylacetyllactosamine; glycoconjugates as virus cell
        adhesion inhibitors)
    75455-20-8DP, conjugates with sialylacetyllactosamine
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (glycoconjugates as virus cell adhesion inhibitors)
    79-10-7D, 2-Propenoic acid, esters, polymers, conjugates with
    sialylacetyllactosamine, biological studies 79-41-4D, esters,
    polymers, conjugates with sialylacetyllactosamine 463-77-4D,
    Carbamic acid, esters, polymers, conjugates with sialylacetyllactosamine,
    biological studies 6703-56-6D, Carbonimidic acid, esters,
    polymers, conjugates with sialylacetyllactosamine 9003-01-4D,
    conjugates with sialylacetyllactosamine 9003-05-8D,
     Polyacrylamide, conjugates with sialylacetyllactosamine 9004-54-0D
     , Dextran, conjugates with sialylacetyllactosamine, biological studies
    9012-72-0D, Glucan, conjugates with sialylacetyllactosamine
    9012-76-4D, Chitosan, conjugates with sialylacetyllactosamine
    25014-12-4D, Polymethacrylamide, conjugates with
    sialylacetyllactosamine 31621-87-1D, Polydioxanone, conjugates
    with sialylacetyllactosamine
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (glycoconjugates as virus cell adhesion inhibitors)
    541-88-8, Chloroacetic anhydride 3655-05-8
    4742-00-1, Tetrakis(aminomethyl)methane 29248-48-4
    32564-25-3, Bis(4-nitrophenyl) adipate 67391-52-0,
     Poly(4-nitrophenyl acrylate) 205753-11-3
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (glycoconjugates as virus cell adhesion inhibitors)
    205753-09-9P 205753-10-2P
ΙT
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (glycoconjugates as virus cell adhesion inhibitors)
    151704-01-7P 205753-07-7P 205830-65-5P
TI
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (glycoconjugates as virus cell adhesion inhibitors)
ΙT
     78969-47-8, 6'-Sialyl-N-acetyllactosamine
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (carrier conjugates; glycoconjugates as virus cell adhesion inhibitors)
RN
     78969-47-8 HCAPLUS
CN
     D-Glucose, O-(N-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-
     qalactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy- (9CI) (CA INDEX
    NAME)
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Absolute stereochemistry.

IT 31621-87-1, Polydioxanone

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(conjugates with sialylacetyllactosamine; glycoconjugates as virus cell adhesion inhibitors)

RN 31621-87-1 HCAPLUS

CN Poly[oxy(1-oxo-1,2-ethanediyl)oxy-1,2-ethanediyl] (9CI) (CA INDEX NAME)

TT 75455-20-8DP, conjugates with sialylacetyllactosamine RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(glycoconjugates as virus cell adhesion inhibitors)

RN 75455-20-8 HCAPLUS

CN 2-Propenamide, N,N-bis(2-hydroxyethyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 10196-26-6 CMF C7 H13 N O3

T79-10-7D, 2-Propenoic acid, esters, polymers, conjugates with sialylacetyllactosamine, biological studies 79-41-4D, esters, polymers, conjugates with sialylacetyllactosamine 463-77-4D,

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Carbamic acid, esters, polymers, conjugates with sialylacetyllactosamine,
     biological studies 6703-56-6D, Carbonimidic acid, esters,
     polymers, conjugates with sialylacetyllactosamine 9003-01-4D,
     conjugates with sialylacetyllactosamine 9003-05-8D,
     Polyacrylamide, conjugates with sialylacetyllactosamine 9004-54-0D
     , Dextran, conjugates with sialylacetyllactosamine, biological studies
     9012-72-0D, Glucan, conjugates with sialylacetyllactosamine
     9012-76-4D, Chitosan, conjugates with sialylacetyllactosamine
     25014-12-4D, Polymethacrylamide, conjugates with
     sialylacetyllactosamine 31621-87-1D, Polydioxanone, conjugates
     with sialylacetyllactosamine
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (glycoconjugates as virus cell adhesion inhibitors)
     79-10-7 HCAPLUS
RN
     2-Propenoic acid (9CI) (CA INDEX NAME)
CN
HO-C-CH=CH_2
RN
     79-41-4 HCAPLUS
CN
     2-Propenoic acid, 2-methyl- (9CI) (CA INDEX NAME)
   CH<sub>2</sub>
Me-C-CO2H
RN
     463-77-4 HCAPLUS
     Carbamic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
CN
HO-C-NH2
     6703-56-6 HCAPLUS
RN
     Carbonimidic acid (9CI) (CA INDEX NAME)
CN
   NH
но-с-он
     9003-01-4 HCAPLUS
RN
CN
     2-Propenoic acid, homopolymer (9CI) (CA INDEX NAME)
     CM
          1
     CRN
         79-10-7
     CMF
         C3 H4 O2
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4742-00-1, Tetrakis(aminomethyl)methane 29248-48-4
32564-25-3, Bis(4-nitrophenyl) adipate 67391-52-0,
Poly(4-nitrophenyl acrylate) 205753-11-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(glycoconjugates as virus cell adhesion inhibitors)
RN 541-88-8 HCAPLUS

CN Acetic acid, chloro-, anhydride (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 3655-05-8 HCAPLUS

RN 4742-00-1 HCAPLUS

CN 1,3-Propanediamine, 2,2-bis(aminomethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 29248-48-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[N-[(1,1-dimethylethoxy)carbonyl]glycylglycyl]oxy ]- (9CI) (CA INDEX NAME)

RN 32564-25-3 HCAPLUS

CN Hexanedioic acid, bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)

RN 67391-52-0 HCAPLUS

CN 2-Propenoic acid, 4-nitrophenyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 2123-85-5 CMF C9 H7 N O4

$$O = C - CH = CH_2$$

$$O_2N$$

RN 205753-11-3 HCAPLUS

CN D-Glucose, O-(N-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy-, ammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 205753-09-9P 205753-10-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(glycoconjugates as virus cell adhesion inhibitors)

RN 205753-09-9 HCAPLUS

CN 2,5,9,12-Tetraazatridecanedioic acid, 7,7-bis[[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]methyl]-4,10-dioxo-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 205753-10-2 HCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]glycylglycyl-, tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

IT 151704-01-7P 205753-07-7P 205830-65-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (glycoconjugates as virus cell adhesion inhibitors)

RN 151704-01-7 HCAPLUS

CN Acetamide, N-[O-(N-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy-.beta.-D-glucopyranosyl]-2-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 205753-07-7 HCAPLUS

CN Hexanoic acid, 6-[[2-[[O-(N-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy-.beta.-D-glucopyranosyl]amino]-2-oxoethyl]amino]-6-oxo-, 1-(4-nitrophenyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

RN 205830-65-5 HCAPLUS
CN Glycine, N-[6-[[2-[[0-(N-acetyl-.alpha.-neuraminosyl)-(2.fwdarw.6)-O-.beta.-D-galactopyranosyl-(1.fwdarw.4)-2-(acetylamino)-2-deoxy-.beta.-D-glucopyranosyl]amino]-2-oxoethyl]amino]-1,6-dioxohexyl]glycylglycyl-,3,3',3'',3'''-tetraamide with 2,2-bis(aminomethyl)-1,3-propanediamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*